

Some Useful Reparameterizations: Linear to Nonlinear Models

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ABSTRACT

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SUMMARY

Quadratic regression models are reparameterized to include either the optimum or the root(s) of the equations as nonlinear parameters. Using nonlinear least squares to fit the reparameterized model yields approximate standard errors and confidence intervals more easily than using the delta method or Fieller's Theorem. Appropriate starting values for nonlinear least squares are readily obtained. In addition, fitting the reparameterized model using nonlinear least squares directly provides an estimate of the standard error of the optimum, which is guaranteed to be the same as that provided by the delta method. These methods are demonstrated with data arising from a quadratic model for stomatal conductance as a function of vapor pressure deficit.

KEY WORDS: Quadratic regression; Interval estimation; Fieller's Theorem, Nonlinear regression; Delta method.

1. INTRODUCTION

The idea of reparameterizing a nonlinear equation to include a parameter of interest often is employed in bioassay to find the ED_{50} associated with a given compound, i.e., the dose of the test substance at which 50% of the organisms respond (Cox, 1990). Reparameterizations in nonlinear models for other applications have been employed for many years as well (Meredith, 1987). Seber and Wild (1989) illustrate reparameterization of nonlinear models to improve convergence and stability of estimates. It is natural to reparameterize a linear model, either full rank or not of full rank, into another linear model. An example in simple linear regression is fitting the mean-slope model versus the intercept-slope model (Snedecor and Cochran, 1980; p. 151). In ANOVA, the overparameterized linear model with overall mean, treatment effects, etc. may be reparameterized more naturally as the full rank cell means model.

However, the practice of reparameterizing linear regression models into nonlinear regression models largely seems to have been overlooked. Perhaps this has been due to the complexities of nonlinear versus linear least squares. Our interest in the reparameterization of a quadratic regression model to include the optimum or the roots, and the use of nonlinear least squares to fit the reparameterized models, was motivated by consulting with plant biologists studying physiological responses to environmental factors. In this paper, we

illustrate the ease of fitting the nonlinear regression model resulting from reparameterization of a quadratic regression model to include explicitly the optimum as a parameter. Appropriate starting values for nonlinear least squares are readily obtained, since one can calculate directly the "correct" answer using the parameter estimates from the linear model fit by ordinary least squares. In addition, fitting the reparameterized model using nonlinear least squares directly provides standard errors and confidence intervals for the parameters of interest, and these are guaranteed to be the same as those provided by the delta method (Cox, 1990; p. 711). Of course, the latter method requires much more labor.

In Section 2, we will discuss the use of quadratic regression models in plant biology and illustrate the use of nonlinear least squares using stomatal conductance data from arctic plants. In this example, the optimum of the quadratic model is the parameter of interest. In Section 4, we will describe briefly how to apply this methodology if the roots of a quadratic equation are the parameters of interest. We also will discuss the confidence interval estimation for the optimum or the roots.

3. Estimation of the Optimum from a Quadratic Regression

The parameterization including the optimum was relevant for modelling

changes in stomatal conductance of arctic plants as a function of diurnal fluctuations in vapor pressure deficit (VPD). Stomatal conductance measures the potential flow of water vapor between the atmosphere and the leaf interior via the stomata, adjustable pores in the leaf surfaces. The relationship was expected to be parabolic, with conductance increasing and then decreasing with increasing time or VPD (Figure 1). Because there are virtually 24 hours of daylight in midsummer within the Arctic Circle, there should be no leveling off of the response in the early morning or in the evening hours. Consequently, a parabolic response curve was the theoretical model rather than an approximation. In this case, the maximum conductance and the VPD value at which the maximum occurred (VPD optimum) were the relevant parameters, used to describe the response of different species. Data from this study will be used below to illustrate the application of nonlinear least squares to estimate the VPD optima for several arctic species.

(Insert Figure 1)

The quadratic regression $Y_i = \alpha + \beta X_i + \gamma X_i^2 + \varepsilon_i$ can be reparameterized as

$$Y_i = \alpha + \gamma X_i (X_i - 2 X_0) + \varepsilon_i \quad (1)$$

to include the optimum of the equation, $X_0 = -\beta / 2\gamma$, which represents the X value at which the maximum (or minimum) response occurs. Using a Taylor series expansion of $-\hat{\beta} / 2\hat{\gamma}$ about (β, γ) , and retaining only terms through second order, the variance of the optimum is approximately given by

$$\text{Var}(\hat{X}_0) \equiv (\hat{\beta} / 2 \hat{\gamma})^2 \left\{ \left(\text{Var}(\hat{\beta}) / \hat{\beta}^2 \right) + \left(\text{Var}(\hat{\gamma}) / \hat{\gamma}^2 \right) - \left(2 \text{Cov}(\hat{\beta}, \hat{\gamma}) / (\hat{\beta} \hat{\gamma}) \right) \right\}. \quad (2)$$

The approximate 95% confidence interval for the optimum, derived using the delta method, is given by:

$$\left((\hat{\beta} / 2 \hat{\gamma}) \pm Z \left((\hat{\beta} / 2 \hat{\gamma})^2 \left[\left(\widehat{\text{Var}}(\hat{\beta}) / \hat{\beta}^2 \right) + \left(\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2 \right) - \left(2 \text{Cov}(\hat{\beta}, \hat{\gamma}) / (\hat{\beta} \hat{\gamma}) \right) \right] \right)^{1/2} \right). \quad (3)$$

An alternative asymmetric interval can be derived using Fieller's Theorem.

Fieller (1954) derived a confidence interval for the ratio of the expected values of two normally-distributed random variables with known variance-covariance matrix, based on the following pivotal quantity, which has a normal distribution:

$$(p - \lambda q) / \left(\text{Var}(p) - 2 \text{Cov}(p, q) + \lambda^2 \text{Var}(q) \right)^{1/2}$$

where P is the random variable in the numerator of the ratio, Q is the random variable in the denominator of the ratio and p and q are estimates of P and Q, and $\lambda = E(P) / E(Q)$, respectively. Equating the pivotal quantity to the critical value of the normal distribution, yields the equation

$$\left[(p/q) - \lambda \right]^2 = \left(\frac{Z}{q / (\text{Var}(q))^{0.5}} \right)^2 \left[(\text{Var}(p) / \text{Var}(q)) - 2 \lambda (\text{Cov}(p, q) / \text{Var}(q)) + \lambda^2 \right] \quad (4)$$

whose roots in λ are the endpoints of the Fieller's interval. Thus, the limits given by Fieller's Theorem represent the intersection points of the two parabolas, whose equations are described by the the right- and left-hand sides of equation (4). Notice that $q / (\text{Var}(q))^{0.5}$ must be large relative to the critical value of the normal distribution, Z, in order to get a confidence interval about λ that is sensible. In practice, the unknown variance of $p - \lambda q$ is estimated using the

residual sum of squares from the regression, and the pivotal quantity has a Student's t-distribution rather than a normal distribution. The Fieller's interval is centered about

$$(p / q) - t^2 \widehat{\text{Cov}}(P, Q) / q^2,$$

where t is the critical value of the appropriate t-distribution. The interval is then rescaled by $1-g$, where $g = t^2 \widehat{\text{Var}}(q) / q^2$. Intervals of this type are used commonly in bioassay for comparing the potency of drugs (Finney, 1978; Cox, 1990). In that context, the numerator of the ratio is the difference in mean potency of two drugs and the denominator is either the common slope of the dose-response curves for the two drugs or the difference in slope of the dose-response curves for the drugs. Fieller's interval has infinite length for $g = 1$ and, for $g > 1$, the interval is exclusive: with probability $1 - \alpha$, the true root lies outside confidence interval. Gleser and Hwang (1987) address the existence of finite length confidence sets and their coverage probabilities for the ratio of regression coefficients from a multiple regression model and point out that the relative distance of the intercept to the origin is a critical feature.

The corresponding interval for the optimum, based on Fieller's Theorem, is given by

$$\left\{ \left[\left(-\hat{\beta} / 2\hat{\gamma} \right) + \left(t^2 \widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma}) / 2\hat{\beta}^2 \right) \pm (t / 2\hat{\gamma}) \left[\widehat{\text{Var}}(\hat{\beta}) + (\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2) (\hat{\beta}^2 - t^2 \widehat{\text{Var}}(\hat{\beta})) \right. \right. \right. \\ \left. \left. \left. - (2\hat{\beta} \widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma}) / \hat{\gamma}) - t^2 (\widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma}) / \hat{\gamma})^2 \right]^{1/2} \right] / [1 - t^2 (\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2)] \right\}. \quad (5)$$

If one uses the orthogonalized version of the quadratic regression model, the covariance of the linear and quadratic coefficients is zero, simplifying (3) and (5). Similarly, for the quadratic regression model on the original X scale, $\text{Cov}(\hat{\beta}, \hat{\gamma}) = 0$ when $\text{Var}(\hat{\gamma}) = 0$ or $\text{Var}(\hat{\beta}) = 0$, which simplifies (3) and (5). For $\text{Cov}(\hat{\beta}, \hat{\gamma}) = 0$, Fieller's interval is no longer recentered. The two intervals will not be equal unless $\text{Var}(\hat{\gamma}) = 0$.

The two intervals have similar length for $\widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma}) = 0$ and small ratio of $\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2$, the square of the estimated coefficient of variation of the curvature. According to Finney (1978; p. 82), the 2 methods yield similar intervals for $g < 0.05$. Empirically, it can be shown that if $\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2$ is less than or equal to 0.02, the lengths of the 2 intervals differ by less than 9% for a wide range of values of the covariance (Table 2). For $\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2$ close to $1/t^2$ (i.e., for g close to 1) and all values of the covariance investigated, the Fieller's interval is much longer than the corresponding Taylor series interval. A critical value of 2.0 was used in all calculations, with the optimum held fixed.

(Insert Table 1)

Figure 1 illustrates the relationship between stomatal conductance and VPD for *Carex aquatilis*, a sedge, which was growing within the Arctic Circle.

Similar parabolic relationships were found for the other species studied. Table 2 gives the standard error and confidence interval for the optimum, from fitting the model given in (1) with nonlinear least squares; they are equal to the

square root of (2) and to (3), respectively. The Fieller's interval for the VPD optimum also has been computed, where possible. An important factor in deciding which interval to use for the optimum of a quadratic is whether a symmetric or an asymmetric confidence interval is more appropriate. In this case, there is no compelling subject matter reason for using an asymmetric interval. In addition, the delta method interval can be computed for all species, whereas the variance of the quadratic coefficient is too large, for some species, to obtain confidence intervals via Fieller's Theorem. For *Carex aquatilis*, both intervals could be calculated: both methods give a similar lower confidence limit, but the upper limit from the delta method is 27% smaller than its Fieller's Theorem counterpart.

4. Estimation of the Roots from a Quadratic Regression

The parameterization including the roots was relevant for modelling seasonal rates of change in concentrations of chemical constituents within the plant tissue as a function of ozone dose applied to the plants. Again, the relationship was expected to be parabolic, with the rates of change in concentration increasing and then decreasing with increasing ozone dose for some chemicals, and the rates of change in concentration decreasing and then increasing with increasing ozone dose for others. One summary of the

quadratic relationship useful to the investigators was the positive root or roots of the quadratic prediction equation. The positive root(s) can be interpreted as the dose(s) for which there is no change in the seasonal rate of change of concentration for the chemical constituent within the plant tissue.

The quadratic regression $Y_i = \alpha + \beta X_i + \gamma X_i^2 + \varepsilon_i$ can be reparameterized as

$$Y_i = \gamma (X_i - r_1)(X_i - r_2) + \varepsilon_i \quad (6)$$

to include the roots of the equation, with $r_1 = [-\beta - (\beta^2 - 4\alpha\gamma)^{1/2}] / 2\gamma$ and $r_2 = [-\beta + (\beta^2 - 4\alpha\gamma)^{1/2}] / 2\gamma$. Recall that the roots represent those values of the independent variable for which the response is zero. Notice that each root is just a linear combination of ratios and rational functions. The variance of the roots

$$\begin{aligned} \text{Var} \left(\left[-\hat{\beta} \pm (\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma})^{1/2} \right] / 2\hat{\gamma} \right) &= \text{Var}(\hat{\beta} / 2\hat{\gamma}) + \text{Var} \left((\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma})^{1/2} / 2\hat{\gamma} \right) \\ &\quad \pm 2 \text{Cov} \left([\hat{\beta} / 2\hat{\gamma}], [(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma})^{1/2} / 2\hat{\gamma}] \right) \end{aligned} \quad (7)$$

can be approximated using Taylor series. The estimate of the first term of the RHS of (7) is approximately equal to

$$\widehat{\text{Var}}(\hat{\beta} / 2\hat{\gamma}) \equiv (\hat{\beta}^2 / 4\hat{\gamma}^2) \left\{ \left(\widehat{\text{Var}}(\hat{\beta}) / \hat{\beta}^2 \right) + \left(\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2 \right) - 2 \widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma}) / (\hat{\beta}\hat{\gamma}) \right\}.$$

The estimate of the second term of the RHS of (7) is approximately

$$\begin{aligned} \widehat{\text{Var}} \left((\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma})^{1/2} / 2\hat{\gamma} \right) &\equiv \left[(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}) / (16\hat{\gamma}^2) \right] \left\{ \left(\widehat{\text{Var}}(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}) / (\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma})^2 \right) \right. \\ &\quad \left. + (4 \widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2) - 2 \widehat{\text{Cov}}(\hat{\gamma}^2, \hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}) / \hat{\gamma}^2 (\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}) \right\}, \end{aligned}$$

where

$$\begin{aligned}\widehat{\text{Var}}\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right) &\equiv 4\hat{\beta}^2\widehat{\text{Var}}(\hat{\beta}) + 16\hat{\gamma}^2\widehat{\text{Var}}(\hat{\alpha}) + 16\hat{\alpha}^2\widehat{\text{Var}}(\hat{\gamma}) \\ &- 8\widehat{\text{Cov}}(\hat{\alpha}, \hat{\gamma})\left[\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right] - 16\hat{\beta}\left[\hat{\gamma}\widehat{\text{Cov}}(\hat{\alpha}, \hat{\beta}) + \hat{\alpha}\widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma})\right]\end{aligned}$$

and

$$\begin{aligned}\widehat{\text{Cov}}\left(\hat{\gamma}^2, \hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right) &\equiv 4\hat{\beta}\hat{\gamma}\widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma}) + (-8\hat{\gamma}^2 + 4\widehat{\text{Var}}(\hat{\gamma}))\widehat{\text{Cov}}(\hat{\alpha}, \hat{\gamma}) \\ &- \widehat{\text{Var}}(\hat{\gamma})\left[\widehat{\text{Var}}(\hat{\beta}) + 8\hat{\alpha}\hat{\gamma}\right].\end{aligned}$$

The covariance in the last term of the RHS of (7) equals zero, if approximated to only zero order terms, and is approximately

$$\begin{aligned}\widehat{\text{Cov}}\left(\left[\hat{\beta}/2\hat{\gamma}\right], \left[\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{1/2}/2\hat{\gamma}\right]\right) &\equiv \widehat{\text{Var}}(\hat{\alpha})\left[-2\hat{\beta}\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-3/2}\right] \\ &+ \widehat{\text{Var}}(\hat{\beta})\left[\left(-3\hat{\beta}/2\hat{\gamma}^2\right)\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-1/2} + \left(\hat{\beta}^3/2\right)\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-3/2}\right] \\ &+ \widehat{\text{Var}}(\hat{\gamma})\left[\left(3\hat{\beta}/\hat{\gamma}^4\right) - 2\hat{\beta}\hat{\alpha}^2\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-3/2}\right] \\ &+ \widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma})\left[\left(-2/\hat{\gamma}^3\right)\left(2\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right) - \left(2/\hat{\gamma}^2\right)\left(1 - \hat{\beta}^2\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-1}\right)\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-1/2}\right] \\ &+ \widehat{\text{Cov}}(\hat{\alpha}, \hat{\beta})\left[\left(-2/\hat{\gamma}\right)\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-1/2}\left(1 - \hat{\beta}^2\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-1}\right)\right] \\ &+ \widehat{\text{Cov}}(\hat{\alpha}, \hat{\gamma})\left[\left(-2\hat{\beta}/\hat{\gamma}\right)\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-1/2}\left((-1/\hat{\gamma}) + 2\hat{\alpha}\left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{-1}\right)\right],\end{aligned}$$

if second order terms are included. If only zero order terms are included, the estimated variances of the two roots are forced to be equal.

The approximate 95% confidence interval for the root, based on the delta method, is given by:

$$\left\{\left[\left(-\hat{\beta} \pm \left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{1/2}\right)/2\hat{\gamma}\right] \pm Z\left(\widehat{\text{Var}}\left(\left[\left(-\hat{\beta} \pm \left(\hat{\beta}^2 - 4\hat{\alpha}\hat{\gamma}\right)^{1/2}\right)/2\hat{\gamma}\right]\right)^{1/2}\right\}. \quad (8)$$

The standard error and confidence interval for the root, from fitting the model

given in (6) with nonlinear least squares, are equal to the square root of (7) and to (8), respectively. Second order terms are included in the estimation of the variance of the roots; thus, the estimated standard errors for the two roots will not be equal, in general. Generalized versions of Fieller's Theorem are available (Cox, 1967; Finney, 1978), if an asymmetric confidence interval is desired.

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Table 1

Lengths of approximate 95% confidence intervals for the optimum of the quadratic equation $\hat{Y}_i = -0.277 + 0.924 X_i + -0.318 X_i^2$, based on Fieller's Theorem. The length of the interval using the delta method was 2.910 for all configurations, although the limits varied.

$\widehat{\text{Var}}(\hat{\gamma})/\hat{\gamma}^2$	g	$\widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma})/\hat{\gamma}^2$	Interval Length		% Relative Length
			Fieller's	Difference	
0.0000	0.000	0.000	2.910	0.000	-0.000
0.0010	0.004	0.000	2.922	-0.012	-0.004
		-0.001	2.918	-0.008	-0.003
		-0.010	2.882	0.028	0.010
		-0.050	2.721	0.189	0.065
0.0025	0.010	0.000	2.939	-0.029	-0.010
		-0.001	2.935	-0.025	-0.009
		-0.010	2.899	0.011	0.004
		-0.050	2.737	0.173	0.059
0.0125	0.050	0.000	3.063	-0.153	-0.053
		-0.001	3.059	-0.149	-0.051
		-0.010	3.021	-0.111	-0.038
		-0.050	2.853	0.057	0.020
0.0250	0.100	0.000	3.233	-0.323	-0.111
		-0.001	3.229	-0.319	-0.110
		-0.010	3.189	-0.279	-0.096
		-0.050	3.011	-0.101	-0.035
0.100	0.400	0.000	4.850	-1.940	-0.667
		-0.001	4.843	-1.933	-0.664
		-0.010	4.783	-1.873	-0.644
		-0.050	4.517	-1.607	-0.552

	0.200	0.800	0.000	14.550	-11.640	-4.000
			-0.001	14.530	-11.620	-3.993
			-0.010	14.350	-11.440	-3.931
			-0.050	13.550	-10.640	-3.656
*	0.043	0.172	-0.100	3.028	-0.118	-0.040

NOTE: The maximum occurs at 1.455. The critical value of 2 was used for all interval length calculations. The % relative length has been calculated as $((\text{Length}_{\text{DM}} - \text{Length}_F) / \text{Length}_{\text{DM}}) \times 100$.

* Using $\widehat{\text{Var}}(\hat{\gamma}) / \hat{\gamma}^2$ and $\widehat{\text{Cov}}(\hat{\beta}, \hat{\gamma}) / \hat{\gamma}^2$ based on the data displayed in Figure 1.

Table 2

Vapor pressure deficit (VPD) optima (i.e., VPD at which maximal conductance occurs), their standard errors and their 95% confidence intervals for the lower leaf surfaces of a few important species in the Prudhoe Bay, Alaska area.

Species	VPD optimum (kPa)	95% Confidence Intervals	
		Delta Method	Fieller's
<i>Salix arctica</i>	1.16 ± 0.12	(0.90, 1.42)	*
<i>S. reticulata</i>	0.70 ± 0.61	(-0.59, 1.99)	*
<i>Carex aquatilis</i>	1.46 ± 0.07	(1.32, 1.59)	(1.35, 2.18)

* The ratio $\hat{\gamma} / SE(\hat{\gamma})$ is too small for these species (e.g., less than 4). Therefore, Fieller's confidence intervals are nonsensical.

List of Figures

Figure 1. Relationship between Stomatal Conductance and Vapor Pressure Deficit in *Carex aquatilis*, a sedge. The predicted response (solid line), approximate 95% confidence bands (dashed lines) and observed values (Δ) for stomatal conductance (cm / sec) are plotted against vapor pressure deficit (kPa). The measurements were taken in mid July on plants growing within the Arctic Circle.

